

Virial relations for ultracold trapped Fermi gases with finite range interactions through the BCS-BEC crossover

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We study the virial relations for ultracold trapped two component Fermi gases^{1,2} in the case of short finite range interactions. Numerical verifications for such relations are reported through the BCS-BEC crossover. As an intermediate step, it is necessary to evaluate the partial derivatives of the many body energy with respect to the inverse of the scattering length and with respect to the interaction range. They are found to have extreme values at the unitary limit. The virial results are used to check the quality of the variational wave function involved in the calculations.

In the absence of interaction, the virial theorem relates the energy per particle of a confined atomic gas with the trapping potential. If that potential is harmonic, the theorem states that the total energy per particle is twice the mean trapping potential energy

$$E = 2E_{tr}. \quad (1)$$

For strongly interacting two component Fermi gases, confined by a harmonic trap in the unitary limit, this relation was also shown to be valid experimentally and theoretically^{3,4}. The first derivation of that theorem considered zero-range interactions and made use of the local density approximation. Further insight on the fundamental basis of this relation revealed several remarking features of the unitary gas such as its scaling properties⁵ or a mapping, using group theory, between the trapped and the free space problem⁶. Recently, the Hellmann-Feynman theorem was used to prove Eq. (1) at the unitary limit^{7,8}, and to generalize the virial relations for finite scattering lengths^{1,2}. In fact, general confinement potentials and finite range interactions can directly be taken into account using a general virial theorem which can be stated as follows²:

Consider a Hamiltonian for a system of N particles with arbitrary statistics:

$$H = H' + U(\vec{r}_1, \dots, \vec{r}_N), \quad (2)$$

where H' and its domain depend on p parameters with length dimensions ℓ_1, \dots, ℓ_p , on \hbar and the mass of the particles. $U(\vec{r}_1, \dots, \vec{r}_N)$ denotes a regular arbitrary function that allows the domains of H and H' to coincide, \vec{r}_i is the position vector for the i -th particle. Then,

$$E = \left\langle U + \frac{1}{2} \sum_{i=1}^N \vec{r}_i \cdot \nabla_{\vec{r}_i} U \right\rangle - \frac{1}{2} \sum_{q=1}^p \ell_q \frac{\partial E}{\partial \ell_q} \quad (3)$$

with E the total energy.

For N particles confined by a harmonic trap, $U = \sum_i^N m(\omega_x^2 |x_i|^2 + \omega_y^2 |y_i|^2 + \omega_z^2 |z_i|^2)/2$ and Eq. (3) becomes:

$$E = 2E_{tr} - \frac{1}{2} \sum_{s=1}^p \ell_s \frac{\partial E}{\partial \ell_s}, \quad (4)$$

where $E_{tr} = \langle U \rangle$ is the trapping potential energy.

In the present article, we study $2N$ fermionic atoms in two equally populated hyperfine states ($N = N_{\uparrow} = N_{\downarrow} = 165$) confined by an isotropic three-dimensional harmonic trap of frequency ω , and interacting through an attractive finite range potential $V = -|V_0|e^{-r/r_v}$. This potential is characterized by two parameters, its strength V_0 and its range r_v . When the kinetic energy of the atoms is low enough, the scattering length is a proper parameter to describe the interacting system. For a given number of s -wave bound states and a given r_v , there is a one-to-one relationship between the strength of the potential V_0 and the scattering length a . We consider the case where at most one bound state is admitted by the potential and find the ground state of the many body Schrödinger equation approximately, via a variational Monte Carlo calculation, for several scattering lengths a and short potential ranges $r_v \ll r_{ho} \equiv \sqrt{\hbar/m\omega}$. We then study the behavior of the total, internal and trapping energy as a function of both length parameters a and r_v to verify Eq. (4). The explicit expression of the Hamiltonian is

$$H = \sum_{i,j=1}^N \frac{p_{\uparrow i}^2 + p_{\downarrow j}^2}{2m} + \frac{1}{2} m \omega^2 (r_{\uparrow i}^2 + r_{\downarrow j}^2) + \sum_{i,j} V_{\uparrow i \downarrow j}, \quad (5)$$

and the corresponding virial relation becomes

$$E = 2E_{tr} - \frac{r_v}{2} \frac{\partial E}{\partial r_v} \Big|_{a=\text{constant}} - \frac{a}{2} \frac{\partial E}{\partial a} \Big|_{r_v=\text{constant}} \quad (6)$$

$$= 2E_{tr} - \frac{r_v}{2} \frac{\partial E}{\partial r_v} \Big|_{a=\text{constant}} + \frac{1}{2a} \frac{\partial E}{\partial (1/a)} \Big|_{r_v=\text{constant}}. \quad (7)$$

In the BEC side of the crossover the total energy E can become extremely large compared to the total energy E in the BCS side due to the contribution of the binding energy of the formed molecules. This fact increases the numerical errors in the evaluation of the derivatives in Eq.(7). In order to isolate this two-body effect from many-body effects, we have found convenient to take into account the behavior of the free space binding energy as follows. The two body problem,

$$\left[\frac{p^2}{2\mu} + V(r) \right] \tilde{\varphi}(\mathbf{r}) = \varepsilon \tilde{\varphi}(\mathbf{r}), \quad \mu = m/2, \quad (8)$$

is analytically solvable for s -states, so that the scattering length is explicitly given by

$$\begin{aligned} a &= r_v \eta(\zeta) \\ &= -2r_v \left[\frac{\pi}{2} \frac{N_0(\zeta)}{J_0(\zeta)} - \log(\zeta/2) - C \right], \end{aligned} \quad (9)$$

with $\zeta = (2r_v \sqrt{|V_0|m/\hbar})$, $C = 0.577215664901\dots$ is the Euler constant and J_ν and N_ν represent the Bessel function of the first and second kind of order ν , respectively. This problem has the following bound states

$$\tilde{\varphi}(r) = \mathcal{N} J_{2r_v \sqrt{|\varepsilon_s^{(r_v)}|} m/\hbar}(y), \quad (10)$$

where \mathcal{N} is a normalization factor and $y = \zeta e^{-r/2r_v}$. The boundary condition at the origin implies $J_{x_s}(\zeta) = 0$, so the corresponding eigenenergies $\varepsilon_s^{(r_v)}$ fulfill the equation

$$2r_v \sqrt{|\varepsilon_s^{(r_v)}|} m/\hbar = x_s. \quad (11)$$

That is, x_s is determined by ζ and

$$\varepsilon_s^{(r_v)} = -\frac{(\hbar x_s)^2}{4mr_v^2}. \quad (12)$$

We shall work with $z_0 < \zeta < z_1$ with z_0 and z_1 the first two zeros of the Bessel function J_0 . Under these conditions, just one bound state is admitted for each positive scattering length a . Given a and r_v and using Eq. (9), we can write

$$x_0 = x_0(\zeta) = x_0 \left(\eta^{-1} \left(\frac{a}{r_v} \right) \right) \equiv w \left(\frac{a}{r_v} \right). \quad (13)$$

As a consequence, the ground state binding energy $\varepsilon_0^{(r_v)}$ of the two interacting particle system in otherwise free space satisfies the equation

$$\begin{aligned} r_v \frac{\partial \varepsilon_0^{(r_v)}}{\partial r_v} \Big|_{a=\text{constant}} &= -2\varepsilon_0^{(r_v)} - 2 \frac{\varepsilon_0^{(r_v)} w'(a/r_v)}{x_0} \frac{a}{r_v} \\ &= -2\varepsilon_0^{(r_v)} - a \frac{\partial \varepsilon_0^{(r_v)}}{\partial a} \Big|_{r_v=\text{constant}}. \end{aligned} \quad (14)$$

Thus, if we define

$$\begin{aligned} \tilde{E} &= \frac{E}{2N} & \text{if } a < 0, \\ &= \frac{E}{2N} - \frac{\varepsilon_0^{(r_v)}}{2} & \text{if } a > 0, \end{aligned} \quad (15)$$

and

$$\langle m\omega^2 R^2 \rangle = \langle \frac{\sum_i^N m\omega(|r_{\uparrow i}|^2 + |r_{\downarrow i}|^2)}{2N} \rangle, \quad (16)$$

the virial relation, Eq. (7), reads

$$\langle m\omega^2 R^2 \rangle = \tilde{E} + \frac{r_v}{2} \frac{\partial \tilde{E}}{\partial r_v} \Big|_{a=\text{constant}} - \frac{1}{2a} \frac{\partial \tilde{E}}{\partial (1/a)} \Big|_{r_v=\text{constant}}. \quad (17)$$

This expression is easier to verify numerically than Eq. (7). Notice that, from a dimensional analysis, equations similar to Eq. (13) can be expected to be valid for other forms of the potential.

Approximate ground state eigenfunctions for the Hamiltonian Eq. (5) were obtained variationally. The trial wave functions used have the Eagles-Leggett form

$$\Psi_{\lambda_{EL}} = \mathcal{A}_{\uparrow} \mathcal{A}_{\downarrow} [\phi(1_{\uparrow}, 1_{\downarrow}) \phi(2_{\uparrow}, 2_{\downarrow}) \dots \phi(N_{\uparrow}, N_{\downarrow})] \quad (18)$$

through the BCS-BEC crossover regime. In this equation, \mathcal{A} denotes the antisymmetrizing operator to be applied to all fermions of each species and

$$\phi(\mathbf{r}_{i\uparrow}, \mathbf{r}_{j\downarrow}) \cong \varphi(r_{i,j}) e^{-\lambda_{EL} |\mathbf{r}_{i\uparrow} + \mathbf{r}_{j\downarrow}|^2/4}, \quad (19)$$

where $\varphi(r_{ij})$ is the s-wave ground state solution of the trapped interacting two body problem

$$\left[\frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 r^2 + V(r) \right] \varphi(r) = \varepsilon \varphi(r). \quad (20)$$

The variational parameter λ_{EL} modulates the optimal shape of the atomic cloud. The evaluation of the mean value of the many body Hamiltonian, Eq.(5), for the Eagles-Leggett trial wave function was done using Monte Carlo techniques that take advantage of the structure of the function¹⁰.

For weak interactions, that is for negative scattering lengths shorter than the mean separation between interacting atoms, lower variational energies are obtained using the length scaled ground state solution of the noninteracting problem (which is a product of Slater determinants) multiplied by a Jastrow correlation function

$$\Psi_{\beta, \lambda_J} = F_{\lambda_J}^J \mathcal{A}_{\uparrow} \prod_{i=1, N} \phi_{\mathbf{n}_{\uparrow i}}^{ho}(\beta \mathbf{r}_{\uparrow i}) \mathcal{A}_{\downarrow} \prod_{i=1, N} \phi_{\mathbf{n}_{\downarrow i}}^{ho}(\beta \mathbf{r}_{\downarrow i}), \quad (21)$$

$$F_{\lambda_J}^J = \exp[-\lambda_J \sum_{i\uparrow, j\downarrow} V(|\mathbf{r}_{i\uparrow} - \mathbf{r}_{j\downarrow}|)]. \quad (22)$$

The scaling factors β and λ_J were taken as variational parameters. For the many body ground state calculation, the inputs of the Slater determinants are the single-particle eigenstates of the noninteracting trapped system $\phi_{\mathbf{n}}^{ho}(\mathbf{r})$, and the set of quantum numbers $\{\mathbf{n}\}$ are chosen to give the lowest energy compatible with Pauli exclusion principle. The Fermi energy ϵ_F derived by this procedure can be used to define an effective Fermi wave number $k_F = \sqrt{2m\epsilon_F}/\hbar$, whose inverse is a natural unit for measuring the scattering length in the many body problem.

The potential ranges used to perform the calculations were in the interval $r_V/r_{ho}\epsilon[0.002, 0.015]$. For each r_V and several scattering lengths through the crossover, upper bounds of the energy \tilde{E} were obtained by optimizing the variational parameters λ_{EL} or λ_J and β according to the trial wave function. The optimization of the numerical subroutines allowed to explore higher statistics with respect to previous calculations⁹ and yield the evaluation of the energy with improved accuracy. In Figures 1 and 2 we illustrate the obtained energies, the vertical size of the plotted points are comparable or higher than the numerical errors. Notice that the resulting curves for the energy dependence on the scattering length for a given range and on the range for a given scattering length show a soft structure that allows a numerical interpolation or even an analytical local fitting curve. These interpolations were used to numerically compute the derivatives necessary to verify the virial relations. The results are illustrated in Figures 3 and 4. A remarkable feature found for all the short interaction ranges explored is that both derivatives, $\partial \tilde{E}/\partial(1/k_F a)$ and $\partial \tilde{E}/\partial r_V$, get an extreme value at unitarity.

In Figure 5, we show a comparison between the trapping energy curve as predicted by the virial relation, Eq.(17) and specific values of that energy evaluated directly from the variational functions for a potential range $r_V = 0.0025 r_{ho}$. Notice that there is good overlap between variational and virial results all over the crossover. The width of the continuous curve corresponds to the numerical errors in its derivation. The main source of error for the trapping

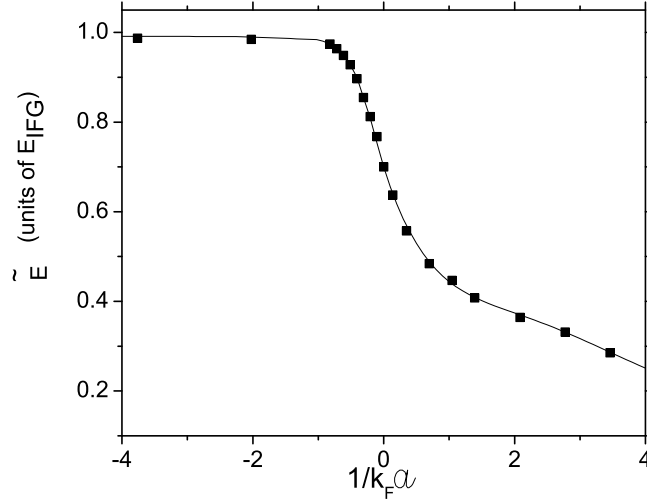


FIG. 1: Many body energy \tilde{E} , Eq.(15), as a function of the inverse of the scattering length for a potential range $r_V = 0.0025r_{ho}$. The energy units correspond to E_{IFG} the energy of the non interacting atomic cloud. The range of the potential is measured in the length scale established by the trapping potential $r_{ho} = \sqrt{\hbar/m\omega}$; k_F denotes the Fermi wave number.

energies evaluated directly from the variational wave functions results from the non uniqueness of the variational parameters λ_{EL} and β that yield similar variational energies. In fact, the agreement between the trapping energy evaluated directly and using the virial relation can be used as an additional criteria to select those parameters. As a reference, in Fig. 5 the many body energy curve $\tilde{E}(1/k_F a)$ is also shown. The crossing of virial $\langle m\omega R^2 \rangle$ and total energy \tilde{E} curves does not occur at unitarity as a finite range effect.

Summarizing, we have studied the virial relations expected for a balanced mixture of two species fermionic trapped atoms interacting through a two parameter (intensity and potential range) attractive potential. We have applied those relations to the study of the ground state solution of this problem when it is approximately obtained using simple form variational trial wave functions. In this way, we are able to quantify the quality of our wave functions and, even more important, we can compare the virial relations of short finite range interaction *versus* contact interactions. Along the calculations, the partial derivatives of the energy \tilde{E} as a function of the scattering length and of the potential range were numerically evaluated. It was found that in all cases considered those derivatives get extreme values at unitarity. As a consequence, an accurate determination of the coefficient \tilde{E}/E_{IFG} at unitarity using finite range potentials require an accurate extrapolation procedure. In a similar way, an accurate experimental determination of such coefficient does require an extremely precise realization of the $1/k_F a \rightarrow 0$ limit.

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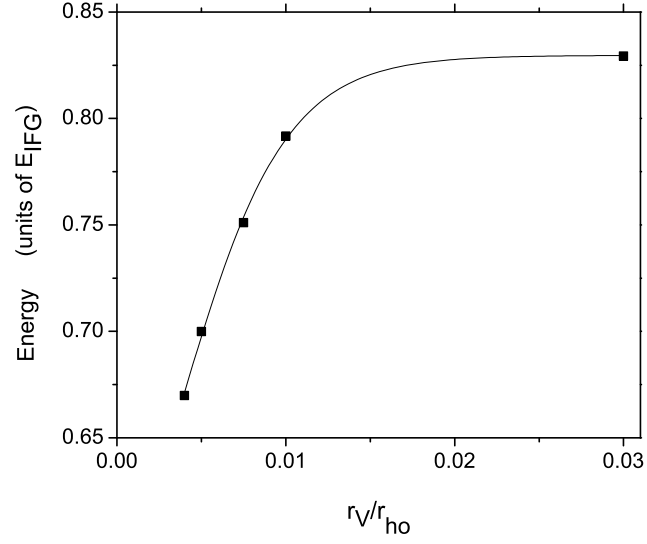


FIG. 2: Many body energy E as a function of the potential range r_V at unitarity, $1/k_F a = 0$. The energy units correspond to E_{IFG} , the energy of the non interacting atomic cloud. The range of the potential is measured in the length scale established by the trapping potential $r_{ho} = \sqrt{\hbar/m\omega}$.

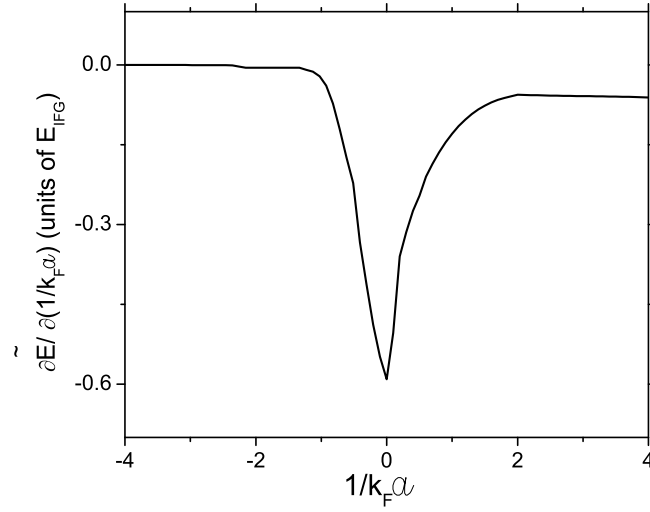


FIG. 3: Partial derivative of the many body energy \tilde{E} , Eq.(15), with respect to the inverse of the scattering length as a function of the inverse of the scattering length for a potential range $r_V = 0.0025 r_{ho}$. The energy units correspond to E_{IFG} , the energy of the non interacting atomic cloud; k_F denotes the Fermi wave number.

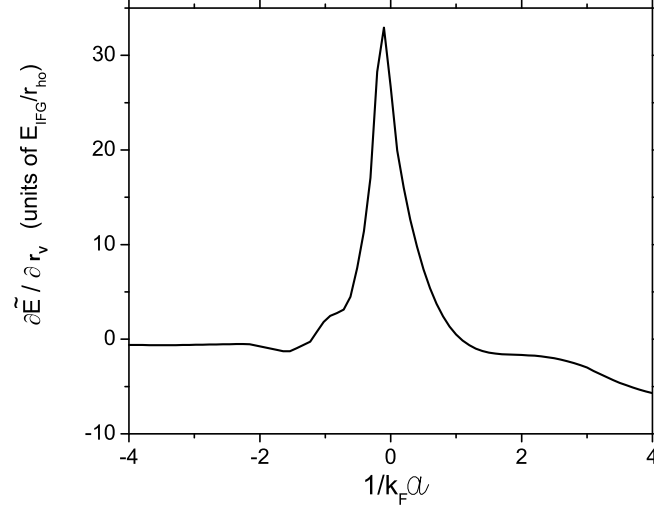


FIG. 4: Partial derivative of the many body energy \tilde{E} with respect to the potential range r_V as a function of the inverse of the scattering length for a potential range $r_V = 0.0025r_{ho}$. The energy units correspond to E_{IFG} , the energy of the non interacting atomic cloud; k_F denotes the Fermi wave number.

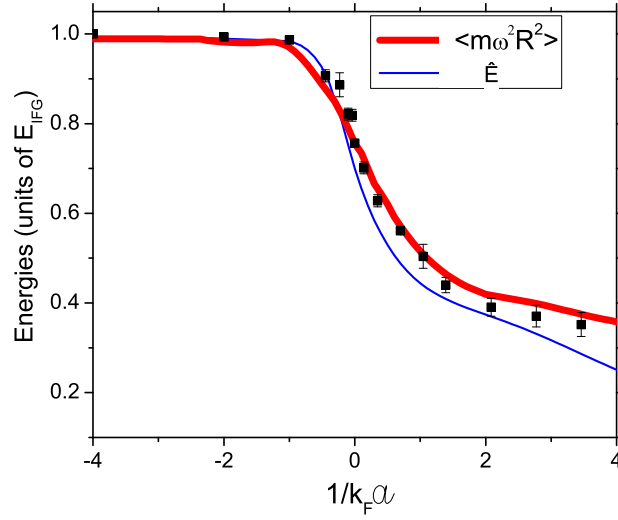


FIG. 5: (Color online) Softened curves for the many body energy \tilde{E} and the mean value of twice the trapping energy $\langle m\omega^2 R^2 \rangle$ as predicted by the virial relation, Eq.(17). The dots represent the value of the trapping energy obtained directly from the variational wave functions. The energy units correspond to E_{IFG} , the energy of the non interacting atomic cloud; k_F denotes the Fermi wave number.